Analytical solutions for the interstitial diffusion of impurity atoms

O. I. Velichko, N. A. Sobolevskaya

Belarusian State University of Informatics and Radioelectronics
Department of Physics, Belarusian State University of Informatics and Radioelectronics,
6, P. Brovki Street, Minsk, 220013 Belarus
E-mail addresses: oleg_velichko@lycos.com (Oleg Velichko)
sobolevskaya@lycos.com (Natalia Sobolevskaya)

Abstract

The analytical solutions of the equations describing impurity diffusion due to migration of nonequilibrium impurity interstitials were obtained for the impurity redistribution during ion implantation at elevated temperatures and for diffusion from a doped epitaxial layer. The reflecting boundary condition at the surface of a semiconductor and the conditions of constant concentrations at the surface and in the bulk of it were used in the first and second cases, respectively. On the basis of these solutions hydrogen diffusion in silicon during high-fluence low-energy deuterium implantation and beryllium diffusion from a doped epi-layer during rapid thermal annealing of InP/InGaAs heterostructures were investigated. The calculated impurity concentration profiles agree well with experimental data. The fitting to the experimental profiles allowed us to derive the values of the parameters that describe interstitial impurity diffusion.

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1 Introduction

The recent years numerical methods have been widely used for simulation of solid state diffusion of ion-implanted dopants (see, for example, [1, 2]). As a rule, to simulate the impurity diffusion a system of equations describing a coupled diffusion of different mobile species and their quasichemical reactions during annealing is solved. Due to a great number of differential equations and the complexity of the system as a whole, the problem of the correctness of a numerical solution is very important. One of the best ways to verify the correctness of an approximate numerical solution is a comparison with the exact analytical solution of the boundary value problem under consideration. Such analytical solutions can be derived for the special simplest cases of dopant or point defect diffusion processes. For example, in Ref. [3] an analytical solution for the point defect diffusion based on the method of Green's functions was obtained. It was supposed in [3] that nonequilibrium point defects were continuously generated during ion implantation of impurity atoms and diffused to the surface and into the bulk of a semiconductor. The surface was considered to be a perfect sink for point defects. In Ref. [4] a process of impurity diffusion during ion implantation at elevated temperatures was investigated analytically. It was supposed that the implantation temperature was too low to provide a traditional

diffusion by the "dopant atom – point defect" pairs, but was enough for the diffusion of nonequilibrium interstitial impurity atoms to occur. Unlike [3], in Ref. [4] a system of equations, namely, the conservation law for substitutionally dissolved impurity atoms and equation of diffusion–recombination of nonequilibrium interstitial impurity atoms have been solved analytically by the method of Green's functions. Reflecting boundary condition at the surface of a semiconductor has been chosen to describe the interaction of interstitial impurity atoms with the interface. Due to this condition, a diffusion problem has become symmetric with respect to the point $x = 0$. For simplicity, the condition of zero impurity concentration for $x \to \pm\infty$ has been used. It is interesting to note that analytical solutions for gold diffusion in silicon due to Frank-Turnbull and due to kick-out mechanisms were obtained in Ref. [5] and Refs. [5, 6], respectively. It was supposed that there was a local equilibrium between substitutionally dissolved impurity atoms, vacancies (or self-interstitials for the kick-out mechanism) and interstitial impurity atoms. The case of nonequilibrium interstitial impurity atoms was not considered in these papers. The very interesting case of coupled diffusion of vacancies and self-interstitials was investigated in [7, 8]. The equations of the diffusion of vacancies or of self-interstitials are similar to the equation of diffusion of impurity interstitials. However, the solutions obtained in [7, 8] are difficult to use for describing the impurity diffusion governed by nonequilibrium interstitial impurity atoms, because a condition of local equilibrium was used in all these papers. Besides, a generation rate was assumed to be equal to zero in [8] or equal to constant value in [7]. Thus, it is reasonable to derive an analytical solution for the case of diffusion due to migration of nonequilibrium impurity interstitials.

The main goal of this paper is to continue the investigation [4] to obtain other analytical solutions and compare these solutions with the experimental data.

2 Original equations

It is supposed that the processing temperature is too low to provide a diffusion of substitutionally dissolved impurity atoms, but is enough for the diffusion of impurity interstitials. The generation of nonequilibrium interstitial impurity atoms can occur due to ion implantation, including the case of ion implantation at elevated temperatures, or due to the replacement of the impurity atom by self-interstitial from the substitutional position to the interstitial one (Watkins effect [9]), or due to dissolution of the clusters that incorporate impurity atoms etc. It is also supposed that the impurity concentration in the doped regions formed due to migration of nonequilibrium impurity interstitials is smaller than n_2 or approximately equal to n_i or that impurity atoms in interstitial position are neutral. Here n_i is the intrinsic carrier concentration at the processing temperature. Then, the system of equations describing the evolution of impurity concentration profiles includes [4]:

(i) a conservation law for substitutionally dissolved impurity atoms:

$$\frac{\partial C(x,t)}{\partial t} = \frac{C^{AI}(x,t)}{\tau^{AI}} + G^{AS}(x,t)\,, \tag{1}$$

(ii) an equation of diffusion for nonequilibrium interstitial impurity atoms:

$$d^{AI}\frac{\partial^2 C^{AI}}{\partial x^2} - \frac{C^{AI}}{\tau^{AI}} + G^{AI}(x,t) = 0\,, \tag{2}$$

or

$$-\left[\frac{\partial^2 C^{AI}}{\partial x^2} - \frac{C^{AI}}{l_{AI}^2}\right] = \frac{\tilde{g}^{AI}(x,t)}{l_{AI}^2}\,, \tag{3}$$

where

$$l_{AI} = \sqrt{d^{AI}\tau^{AI}}\,, \qquad \tilde{g}^{AI}(x,t) = G^{AI}(x,t)\,\tau^{AI}\,. \tag{4}$$

Here C and C^{AI} are the concentrations of substitutionally dissolved impurity atoms and nonequilibrium impurity interstitials, respectively; G^{AS} is the rate of introducing of impurity atoms, which immediately occupy the substitutional positions; d^{AI} and τ^{AI} are the diffusivity and average lifetime of nonequilibrium interstitial impurity atoms, respectively; G^{AI} is the generation rate of interstitial impurity atoms. We use a steady-state diffusion equation for impurity interstitials, because of the large average migration length of nonequilibrium interstitial impurity atoms ($l_{AI} \gg l_{fall}$, where l_{fall} is the characteristic length of the decrease in the impurity concentration) and due to the small average lifetime of nonequilibrium impurity interstitials ($\tau_{AI} \ll t_P$, where t_P is the duration of thermal treatment).

The system (1), (2) or (1), (3) describes impurity diffusion due to migration of nonequilibrium interstitial impurity atoms. To solve this system of equations, appropriate boundary conditions are need. Let us consider, in contrast to [4], the finite-length one-dimensional (1D) domain $[0, x_B]$, i.e., the domain used in 1D numerical modeling, and add the following boundary conditions to Eq. (3):

$$\mathrm{w}_1^S d^{AI}\left.\frac{\partial C^{AI}}{\partial x}\right|_{x\,=\,0} + \mathrm{w}_2^S\, C^{AI}\big|_{x\,=\,0} = \mathrm{w}_3^S\,, \tag{5}$$

$$\mathrm{w}_1^B d^{AI}\left.\frac{\partial C^{AI}}{\partial x}\right|_{x\,=\,x_B} + \mathrm{w}_2^B\, C^{AI}\big|_{x\,=\,x_B} = \mathrm{w}_3^B\,, \tag{6}$$

as well as the initial conditions:

$$C(x,0) = C_0(x)\,, \qquad C^{AI}(x,0) = C^{AI}_{eq} = const\,. \tag{7}$$

Here, w_1^S, w_2^S, w_3^S and w_1^B, w_2^B, w_3^B are constant coefficients; C^{AI}_{eq} is the equilibrium value of concentration of interstitial impurity atoms (it is supposed that C^{AI}_{eq} is equal to zero for many cases under consideration).

To derive an analytical solution of this boundary value problem, the method of Green's function [10] can be used.

3 Analytical method and solutions

The suggestion about the immobile substitutionally dissolved impurity atoms allows one to solve Eq. (1) independently of Eq. (2) or Eq. (3):

$$C(x,t) = \frac{1}{\tau^{AI}} \int\limits_0^t C^{AI}(x,t)dt + \int\limits_0^t G^{AS}(x,t)dt + C_0(x)\,. \tag{8}$$

We will supplement expression (8) with a steady-state solution of Eq. (3) obtained by the method of Green's functions [10]:

$$C^{AI}(x,t) = \int\limits_0^{x_B} G(x,\xi) w(\xi,t) d\xi\,, \tag{9}$$

where

$$w(\xi,t) = \frac{\tilde{g}^{AI}(\xi,t)}{l_{AI}^2} + w_S(\xi) + w_B(\xi)\,. \tag{10}$$

Here $G(x,\xi)$ is the Green's function for Eq. (3). Using the standardizing function $w(x,t)$ [10] allows one to reduce the previous boundary value problem to the boundary value problem with zero boundary conditions:

$$\mathrm{w}_1^S d^{AI} \left.\frac{\partial C^{AI}}{\partial x}\right|_{x\,=\,0} + \mathrm{w}_2^S \left. C^{AI}\right|_{x\,=\,0} = 0\,, \tag{11}$$

$$\mathrm{w}_1^B d^{AI} \left.\frac{\partial C^{AI}}{\partial x}\right|_{x\,=\,x_B} + \mathrm{w}_2^B \left. C^{AI}\right|_{x\,=\,x_B} = 0\,. \tag{12}$$

The Green's function for Eq. (3) with boundary conditions (11) and (12) has the following form [10]:

$$G(x,\xi) = \frac{1}{K} \begin{cases} Q_1(x)Q_2(\xi) & \text{for } 0 \le x \le \xi \le x_B\,, \\ Q_1(\xi)Q_2(x) & \text{for } 0 \le \xi \le x \le x_B\,, \end{cases} \tag{13}$$

where

$$K = Q_1^{'}(x)Q_2(x) - Q_1(x)Q_2^{'}(x) = const\,. \tag{14}$$

Here Q_1 and Q_2 are the linearly independent solutions of the homogeneous equation

$$\frac{\mathrm{d}^2 Q}{\mathrm{d}\, x^2} - \frac{Q}{l_{AI}^2} = 0 \tag{15}$$

with the following initial conditions on the left boundary:

$$Q_1(0) = \mathrm{w}_1^S d^{AI}\,, \qquad Q_1^{'}(0) = -\mathrm{w}_2^S\,, \tag{16}$$

and on the right one:

$$Q_2(x_B) = \mathrm{w}_1^B d^{AI}\,, \qquad Q_2^{'}(x_B) = -\mathrm{w}_2^B\,. \tag{17}$$

Following [10], one can write the functions $w_S(x)$ and $w_B(x)$ as

$$
w_S(x) = \begin{cases} -\dfrac{1}{\mathrm{w}_1^S d^{AI}}\delta(-x)\mathrm{w}_3^S & \text{if } \mathrm{w}_1^S \neq 0\,, \\ \\ \dfrac{1}{\mathrm{w}_2^S}\delta^{'}(-x)\mathrm{w}_3^S & \text{if } \mathrm{w}_2^S \neq 0\,, \end{cases} \tag{18}
$$

$$
w_B(x) = \begin{cases} \dfrac{1}{\mathrm{w}_1^B d^{AI}}\delta(x_B - x)\mathrm{w}_3^B & \text{if } \mathrm{w}_1^B \neq 0\,, \\ \\ -\dfrac{1}{\mathrm{w}_2^B}\delta^{'}(x_B - x)\mathrm{w}_3^B & \text{if } \mathrm{w}_2^B \neq 0\,. \end{cases} \tag{19}
$$

Thus, for the reflecting boundary condition

$$
\mathrm{w}_1^S = 1, \qquad \mathrm{w}_2^S = 0, \qquad \mathrm{w}_3^S = 0 \tag{20}
$$

at the surface of a semiconductor ($x = 0$) and for Dirichlet boundary condition

$$
\mathrm{w}_1^B = 0, \qquad \mathrm{w}_2^B = 1, \qquad \mathrm{w}_3^B = C_B^{AI} \tag{21}
$$

in the bulk ($x = x_B$) the solutions Q_1 and Q_2 have the form

$$
Q_1(x) = d^{AI}\cosh\left(\frac{x}{l_{AI}}\right)\,, \qquad Q_2(x) = l_{AI}\sinh\left(\frac{x_B - x}{l_{AI}}\right)\,, \tag{22}
$$

$$
K = d^{AI}\cosh\left(\frac{x_B}{l_{AI}}\right) = const\,. \tag{23}
$$

$$
G(x,\xi) = \frac{l_{AI}}{\cosh\left(\dfrac{x_B}{l_{AI}}\right)} \begin{cases} \cosh\left(\dfrac{x}{l_{AI}}\right)\sinh\left(\dfrac{x_B - \xi}{l_{AI}}\right) & \text{for } 0 \leq x \leq \xi \leq x_B\,, \\ \\ \cosh\left(\dfrac{\xi}{l_{AI}}\right)\sinh\left(\dfrac{x_B - x}{l_{AI}}\right) & \text{for } 0 \leq \xi \leq x \leq x_B\,, \end{cases} \tag{24}
$$

$$
w_S(x) = 0, \qquad w_B(x) = \delta^{'}(x_B - x)C_B^{AI}\,. \tag{25}
$$

Let us consider the process of ion implantation in a semiconductor at an elevated temperature (the so-called “hot” implantation). It is established experimentally that the main part of the implanted impurity atoms occupies substitutional positions near the places where they were stopped. Let us suppose that the remaining nonequilibrium atoms occupy interstitial sites and can diffuse during implantation before they transfer to the substitutional position. To describe the spatial distributions of both impurity atoms directly occupying substitutional position and impurity interstitials generated during implantation, Gaussian distributions can be used:

$$
G^{AS}(x,t) = g_m(1 - p^{AI})\exp\left[-\frac{(x - R_p)^2}{2\triangle R_p^2}\right]\,, \tag{26}
$$

$$
G^{AI}(x,t) = g_m p^{AI}\exp\left[-\frac{(x - R_p)^2}{2\triangle R_p^2}\right]\,, \tag{27}
$$

where g_m is the number of impurity atoms being introduced per unit area per second by ion implantation; p^{AI} is a part of the implanted impurity atoms occupying interstitial sites; R_p and $\triangle R_p$ are the average projective range of implanted ions and straggling of projective range, respectively.

Taking into consideration expressions (25) and (27) yields

$$w(\xi,t) = \frac{g_m p^{AI} \tau^{AI}}{l_{AI}^2} \exp\left[-\frac{(\xi - R_p)^2}{2\triangle R_p^2}\right] - \delta^{'}(x_B - \xi) C_B^{AI} \,. \tag{28}$$

Substituting Green's function (24) and standardizing function (28) into expression (9) allow one to obtain a spatial distribution of diffusing interstitial impurity atoms:

$$\begin{aligned} C^{AI}(x,t) = \int\limits_0^{x_B} G(x,\xi) w(\xi,t) d\xi = \frac{g_m p^{AI} \tau^{AI}}{l_{AI}} \cosh^{-1}\left(\frac{x_B}{l_{AI}}\right) \\ \times \left\{ \sinh\left(\frac{x_B - x}{l_{AI}}\right) \int\limits_0^{x} \cosh\left(\frac{\xi}{l_{AI}}\right) \exp\left[-\frac{(R_p - \xi)^2}{2\triangle R_p^2}\right] d\xi \right. \\ \left. + \cosh\left(\frac{x}{l_{AI}}\right) \int\limits_x^{x_B} \sinh\left(\frac{x_B - \xi}{l_{AI}}\right) \exp\left[-\frac{(R_p - \xi)^2}{2\triangle R_p^2}\right] d\xi \right\} \\ + C_B^{AI} \cosh^{-1}\left(\frac{x_B}{l_{AI}}\right) \cosh\left(\frac{x}{l_{AI}}\right) \int\limits_x^{x_B} \sinh\left(\frac{\xi - x_B}{l_{AI}}\right) \delta^{'}(x_B - \xi) d\xi \,. \end{aligned} \tag{29}$$

Calculating the integrals on the right-hand side of expression (29) one can obtain an explicit expression for the distribution of interstitial impurity atoms:

$$\begin{aligned} C^{AI}(x,t) = C_m \frac{\exp\, u_1}{\cosh\, u_2^B} \{ \cosh u_2 [\exp(-u_6)(\mathrm{erf} u_4^B - \mathrm{erf} u_4) \\ + \exp(u_6)(\mathrm{erf} u_5^B - \mathrm{erf} u_5)] + \exp(-u_9) \sinh u_3 \\ \times [\mathrm{erf} u_7 + \exp(2u_9)(\mathrm{erf} u_5 - \mathrm{erf} u_8) - \mathrm{erf} u_4] \} + C_B^{AI} \frac{\cosh u_2}{\cosh u_2^B} \,, \end{aligned} \tag{30}$$

where

$$C_m = \frac{\sqrt{\pi} g_m p^{AI} \tau^{AI} \Delta R_p}{2\sqrt{2}\, l_{AI}} \,, \tag{31}$$

$$u_1 = \frac{\Delta R_p^2}{2 l_{AI}^2} \,, \tag{32}$$

$$u_2 = \frac{x}{l_{AI}} \,, \qquad u_2^B = \frac{x_B}{l_{AI}} \,, \tag{33}$$

$$u_3 = \frac{x - x_B}{l_{AI}} \,, \tag{34}$$

$$u_4 = \frac{\Delta R_p^2 - l_{AI} R_p + l_{AI} x}{\sqrt{2}\Delta R_p l_{AI}} \,, \qquad u_4^B = \frac{\Delta R_p^2 - l_{AI} R_p + l_{AI} x_B}{\sqrt{2}\Delta R_p l_{AI}} \,, \tag{35}$$

$$u_5 = \frac{\Delta R_p^2 + l_{AI} R_p - l_{AI} x}{\sqrt{2}\Delta R_p l_{AI}} \,, \qquad u_5^B = \frac{\Delta R_p^2 + l_{AI} R_p - l_{AI} x_B}{\sqrt{2}\Delta R_p l_{AI}} \,, \tag{36}$$

$$u_6 = \frac{R_p - x_B}{l_{AI}} \,, \tag{37}$$

$$u_7 = \frac{\Delta R_p^2 - l_{AI} R_p}{\sqrt{2}\Delta R_p l_{AI}} \,, \qquad u_8 = \frac{\Delta R_p^2 + l_{AI} R_p}{\sqrt{2}\Delta R_p l_{AI}} \,, \tag{38}$$

$$u_9 = \frac{R_p}{l_{AI}} \,. \tag{39}$$

In a similar way, one can obtain a solution for the case of impurity interstitial recombination at the surface of a semiconductor. Let us consider, for example, a buried layer uniformly doped by impurity atoms. If the impurity concentration is high, generation of nonequilibrium interstitial impurity atoms is possible within this layer during thermal treatment. The boundary conditions assuming the constant impurity interstitial concentrations at the surface and in the bulk of a semiconductor (Dirichlet boundary conditions) can be enforced to describe the interstitial migration

$$C^{AI}\big|_{x\,=\,0} = C_S^{AI} \,, \qquad C^{AI}\big|_{x\,=\,x_B} = C_B^{AI} \,, \tag{40}$$

where C_S^{AI} is the concentration of interstitial impurity atoms at the surface (it is quite likely that $C_S^{AI} = 0$).

Let us suppose that the generation of impurity interstitials is described by the following function:

$$G^{AI}(x) = \begin{cases} 0 & \text{for } 0 \leq x < x_L \,, \\ g_m & \text{for } x_L \leq x \leq x_R \,, \\ 0 & \text{for } x_R < x \leq x_B \,, \end{cases} \tag{41}$$

where $g_m = const$ and x_L and x_R are the left and right boundaries of the doped layer, respectively.

Then, the Green's function and standardizing function are respectively

$$G(x,\xi) = \frac{l_{AI}}{\sinh\left(\dfrac{x_B}{l_{AI}}\right)} \begin{cases} \sinh\left(\dfrac{x}{l_{AI}}\right) \sinh\left(\dfrac{x_B - \xi}{l_{AI}}\right) & \text{for } 0 \leq x \leq \xi \leq x_B \,, \\ \sinh\left(\dfrac{\xi}{l_{AI}}\right) \sinh\left(\dfrac{x_B - x}{l_{AI}}\right) & \text{for } 0 \leq \xi \leq x \leq x_B \,, \end{cases} \tag{42}$$

and

$$w(\xi,t)=\frac{G_{AI}(\xi)\,\tau^{AI}}{l_{AI}^2}-\delta^{'}(-\xi)C_S^{AI}-\delta^{'}(x_B-\xi)C_B^{AI}\,. \tag{43}$$

Substituting (41), (42), and (43) into expression (9), we obtain a spatial distribution of the diffusing interstitial impurity atoms:

$$C^{AI}(x,t)=C^{AI}(x)=C_p^{AI}(x)+C_h^{AI}(x)\,, \tag{44}$$

where

$$\begin{gathered}C_p^{AI}(x)=\frac{\tau^{AI}}{l_{AI}}\sinh^{-1}\left(\frac{x_B}{l_{AI}}\right)\left[\sinh\left(\frac{x_B-x}{l_{AI}}\right)\int\limits_0^x\sinh\left(\frac{\xi}{l_{AI}}\right)G_{AI}(\xi)d\xi\right.\\ \left.+\sinh\left(\frac{x}{l_{AI}}\right)\int\limits_x^{x_B}\sinh\left(\frac{x_B-\xi}{l_{AI}}\right)G_{AI}(\xi)d\xi\right]\,,\end{gathered} \tag{45}$$

$$\begin{aligned}C_h^{AI}(x)&=-C_S^{AI}\int\limits_0^{x_B}G(x,\xi)\delta^{'}(-\xi)d\xi-C_B^{AI}\int\limits_0^{x_B}G(x,\xi)\delta^{'}(x_B-\xi)d\xi\\ &=\sinh^{-1}\left(\frac{x_B}{l_{AI}}\right)\left[C_S^{AI}\sinh\left(\frac{x_B-x}{l_{AI}}\right)+C_B^{AI}\sinh\left(\frac{x}{l_{AI}}\right)\right]\,.\end{aligned} \tag{46}$$

To calculate the integrals in expression (45), let us consider the following three cases:
i) If $x<x_L$, then

$$\begin{gathered}C_p^{AI}(x)=\frac{\tau^{AI}g_m}{l_{AI}}\sinh\left(\frac{x}{l_{AI}}\right)\int\limits_{x_L}^{x_R}\sinh\left(\frac{x_B-\xi}{l_{AI}}\right)d\xi=\tau^{AI}g_m\\ \times\sinh^{-1}\left(\frac{x_B}{l_{AI}}\right)\sinh\left(\frac{x}{l_{AI}}\right)\left[\cosh\left(\frac{x_B-x_L}{l_{AI}}\right)-\cosh\left(\frac{x_B-x_R}{l_{AI}}\right)\right]\,,\end{gathered} \tag{47}$$

ii) If $x_L\le x\le x_R$, then

$$\begin{gathered}C_p^{AI}(x)=\frac{g_m\,\tau^{AI}}{l_{AI}}\sinh^{-1}\left(\frac{x_B}{l_{AI}}\right)\left[\sinh\left(\frac{x_B-x}{l_{AI}}\right)\int\limits_{x_L}^{x}\sinh\left(\frac{\xi}{l_{AI}}\right)d\xi+\right.\\ \left.+\sinh\left(\frac{x}{l_{AI}}\right)\int\limits_x^{x_R}\sinh\left(\frac{x_B-\xi}{l_{AI}}\right)d\xi\right]\\ =g_m\,\tau^{AI}\sinh^{-1}\left(\frac{x_B}{l_{AI}}\right)\left\{\sinh\left(\frac{x_B-x}{l_{AI}}\right)\left[\cosh\left(\frac{x}{l_{AI}}\right)-\cosh\left(\frac{x_L}{l_{AI}}\right)\right]\right.\\ \left.+\sinh\left(\frac{x}{l_{AI}}\right)\left[\cosh\left(\frac{x_B-x}{l_{AI}}\right)-\cosh\left(\frac{x_B-x_R}{l_{AI}}\right)\right]\right\}\,,\end{gathered} \tag{48}$$

iii) If $x > x_R$, then

$$C_p^{AI}(x) = \frac{\tau^{AI} g_m}{l_{AI}} \sinh\left(\frac{x_B - x}{l_{AI}}\right) \int\limits_{x_L}^{x_R} \sinh\left(\frac{\xi}{l_{AI}}\right) d\xi$$

$$= \tau^{AI} g_m \sinh^{-1}\left(\frac{x_B}{l_{AI}}\right) \sinh\left(\frac{x_B - x}{l_{AI}}\right) \left[\cosh\left(\frac{x_R}{l_{AI}}\right) - \cosh\left(\frac{x_L}{l_{AI}}\right)\right] . \tag{49}$$

Expressions (47), (48), and (49) are the partial steady-state solution of the boundary value problem under consideration for the case of step distribution of interstitial generation rate (41) and zero concentrations of nonequilibrium impurity interstitials on the left and right boundaries of the solution domain. Combining these expressions with solution (46) of the appropriate homogeneous diffusion equation, we obtain the distribution of impurity interstitial concentration for the case of the arbitrary boundary concentrations of impurity interstitial atoms (see expression (44)).

4 Simulation

Using the system of Eqs. (1) and (3) and appropriate analytical solutions, one can verify the correctness of numerical calculations. This system can be also used for modeling hydrogen diffusion in silicon. For the case of hydrogen diffusion, the quantities C and C^{AI} are the concentration of trapped (immobile) hydrogen atoms and concentration of the neutral mobile hydrogen interstitials, respectively. As example, in Fig. 1 the results of simulation of hydrogen diffusion in silicon obtained on the basis of analytical solution (8) and (30) are presented. For comparison, the experimental data of [11] are used. In [11] deuterium was introduced in the laser recrystallized silicon ribber by high-fluence low-energy (1.5 keV) ion implantation at a temperature of 250 °C. The deuterium concentration profile presented in Fig. 1 was measured by secondary ion mass spectrometry (SIMS). As can be seen from Fig. 1, the analytical solution obtained provides good agreement with the experimental data [11]. The following values of simulation parameters were used to fit the calculated curve to the experimental deuterium profile: $Q = 4.32{\times}10^{15}$ cm^{-2}; $p^{AI} = 0.253$; $R_P = 0.035$ μm; $\triangle R_P = 0.028$ μm; $l^{AI} = 0.31$ μm. Here Q is the fluence of implanted hydrogen. Thus, it follows from the value of the fitting parameter p^{AI} that approximately 25% of the implanted deuterium atoms occupy interstitial positions. Migration of these nonequilibrium interstitial atoms results in the formation of extended "tail" on the deuterium concentration profile.

In Fig. 2 the beryllium concentration profile after annealing calculated on the basis of analytical solution (8), (47), (48), and (49) is shown. For comparison, the experimental data of [12] are used. In Ref. [12] beryllium diffusion in InGaAs/InP during rapid annealing at a temperature of 900 °C for 30 s was investigated. In the experiment under consideration, InP/InGaAs heterostructures were grown by gas-source molecular beam epitaxy onto semi-insulating ⟨100⟩ InP substrates. At first a 0.1 μm InP buffer layer was grown, followed by 0.5 μm undoped InP and then 0.2 μm Be-doped $In_{0.53}Ga_{0.47}As$ layer with a doping level of $3{\times}10^{7}$ μm^{-3} was grown. Finally, an undoped InP layer of 0.5 μm was grown on the Be doped layer. Then, a post-growth rapid thermal annealing

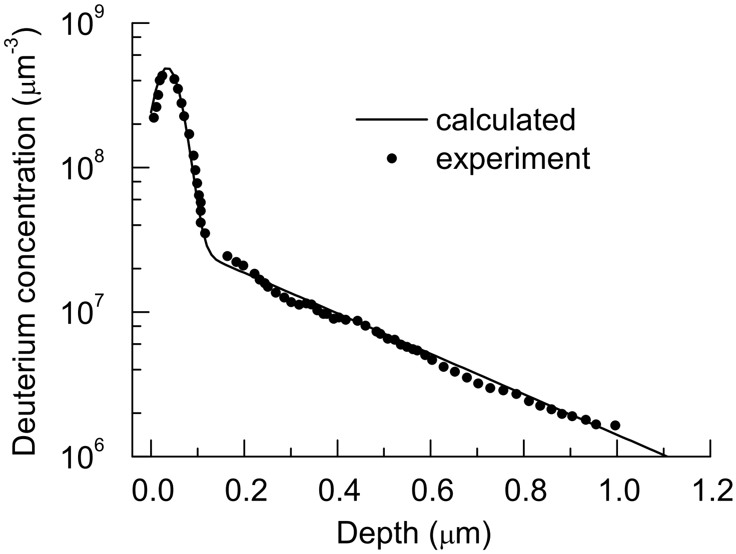

Figure 1: Deuterium concentration profile (solid line) calculated for the case of "hot" ion implantation at a temperature of 250 °C. The experimental data (dots) are taken from Sopori *et al.* [11].

was performed in a halogen lamp furnace for 30 s. Beryllium profile measurements were made with SIMS. The measurements confirmed that the as-grown beryllium concentration profile is a step function, similar to the function (41).

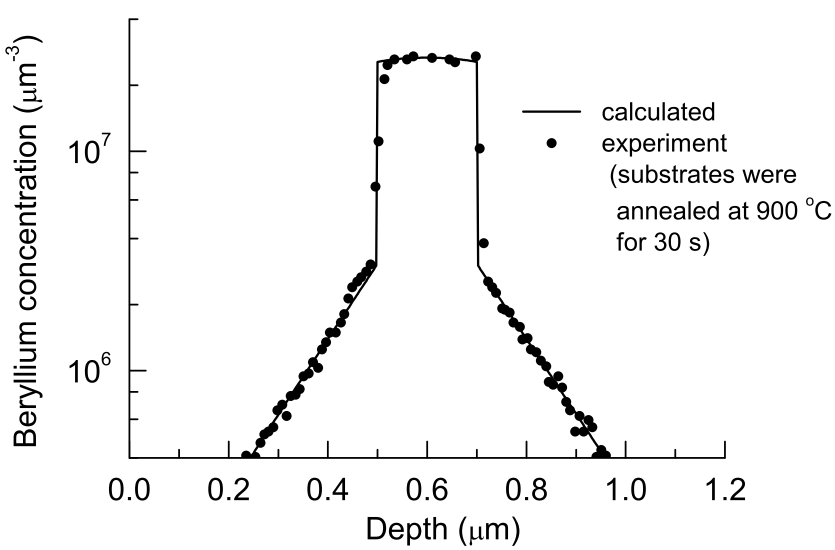

Figure 2: Beryllium concentration profile (solid line) calculated for the case of rapid thermal annealing (30 s at a temperature of 900 °C) of the InP/InGaAs heterostructures. The experimental data (dots) are taken from Ihaddadene-Lenglet *et al.* [12].

To calculate the beryllium concentration profile after annealing it is supposed that during thermal treatment a part of substitutionally dissolved impurity atoms is transferred into interstitial positions. If the generation rate of beryllium interstitials is proportional to the impurity concentration, we can use function (41) to describe the distribution of the interstitial generation rate. It is also supposed that the impurity interstitial concentrations at the surface and in the bulk of a semiconductor are equal to zero. Then, the beryllium concentration profile after annealing is described by analytical expressions (1), (47), (48), and (49).

As can be seen from Fig. 2, the calculated curve is in good agreement with the experimental data of [12]. The following values of simulation parameters were used to fit the calculated curve to the experimental concentration profile of beryllium: $C_{max} = 2.672.\times 10^{7}$ μm^{-3}; $p^{AI} = 0.254$; $x_L = 0.5$ μm; $x_R = 0.7$ μm; $l^{AI} = 0.127$ μm. Here C_{max} is the maximum concentration of substitutionally dissolved beryllium after annealing. It follows from the value of the fitting parameter p^{AI} that, as in the case of "hot" ion implantation, approximately 25% of the beryllium atoms occupy the transient interstitial positions. Migration of these nonequilibrium impurity interstitial atoms results in the formation of two "tails" on the beryllium concentration profile after annealing.

5 Conclusions

The analytical solutions of the equations describing impurity diffusion due to migration of nonequilibrium impurity interstitials are obtained. Two representative cases were investigated: i) interstitial impurity diffusion during "hot" ion implantation under reflecting boundary condition at the surface of a semiconductor; ii) impurity interstitial diffusion from the doped epitaxial layer under the conditions of constant concentrations of interstitial impurity atoms at the surface and in the bulk.

Using these solutions, we can verify the correctness of the approximate numerical calculations obtained by the codes intended for simulation of diffusion processes used in fabrication of semiconductor devices. Moreover, it is possible to carry out an analytical simulation of certain diffusion processes. As an example, hydrogen diffusion in silicon during high-fluence low-energy deuterium implantation at a temperature of 250 °C and beryllium diffusion from a doped epi-layer during rapid thermal annealing of InP/InGaAs heterostructures at a temperature of 900 °C were investigated. The impurity concentration profiles calculated on the basis of the analytical solutions obtained agree well with the experimental data. Due to comparison with experiment, the values of the parameters describing interstitial impurity diffusion have been derived. It was obtained that for the processes under consideration approximately 25% of the impurity atoms occupied transient interstitial positions. The average migration lengths of impurity interstitials are 0.31 and 0.127 μm for deuterium in silicon and beryllium in InP, respectively.

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